Pyrazine, 2,3-dimethyl-5-(2-methylpropyl)-

Other names:	5-Isobutyl-2,3-dimethylpyrazine
	2,3-Dimethyl-5-isobutylpyrazine
	Pyrazine, 2,3-dimethyl-5-isobutyl
Inchi:	InChI=1S/C10H16N2/c1-7(2)5-10-6-11-8(3)9(4)12-10/h6-7H,5H2,1-4H3
InchiKey:	HPAYBTQBMQPWCN-UHFFFAOYSA-N
Formula:	C10H16N2
SMILES:	Cc1ncc(CC(C)C)nc1C
Mol. weight [g/mol]:	164.25
CAS:	54410-83-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.35		Crippen Method
logp	2.292		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
rinpol	1200.00		NIST Webbook
ripol	1558.00		NIST Webbook
ripol	1525.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54410832&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

rinpol: Non-polar retention indices

ripol: Polar retention indices

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